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Evaluation of Tentative Terminations in New Chemical Review

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I. Summary

As the TSCA Section 5 chemical review process matures, it has become more and more evident that many substances are not expected to pose concerns for the Office of Toxic Substances. If we could identify these substances early and terminate their review, resources could be concentrated on the substances that appear to pose concerns and, therefore, benefit more from further assessment.

This paper documents additional criteria that would permit more "drops" to be made at the Chemistry Review and Search Strategy (CRSS) meeting. We describe three modified criteria and one new criterion that can be integrated into our existing CRSS drop approach. We developed these additional criteria from data we compiled for a series of cases that CRSS predicted would be dropped at the Focus meeting. The Structure/Activity Team (SAT) was also asked to make these predictions. In 98 percent of the cases, these predictions were correct.

We also suggest work that could lead to a future approach consisting of new kinds of criteria and a new framework from which criteria may be applied.

Based on past experience, the recommendations we propose should increase CRSS drops from about 20 percent to about 27* percent of all cases. Although the actual incidence of CRSS

*This computation is based upon an analysis performed using a draft version of the new criteria. The current proposal includes changes that may act in opposing directions. The net result, in our opinion, is likely to be either no change or a modest increase in the incidence of drops.

drops will depend on the nature of substances submitted and other developments, we believe that with a new approach based on further work in the future we could expect the number of drops to increase to more than 33 percent of all cases.

II. Background

A. Description of the Objective

The primary objective of this work is to expand the scope of chemical substances for which new chemical review can be efficiently and reliably terminated. A secondary objective is to suggest future work that tentatively identifies new criteria and a new framework on which further expansion could be based.

As early as 1981, resource shortages led an interdivisional OTS group to institute various kinds of case terminations or "drops" from the PMN Review Process. Over the years, many of these policies either have been formalized as exemptions or have been abandoned. Drops for polymers, however, have continued. The Industrial Chemistry Branch (ICB) terminates certain polymers from review at the ICB Chemistry Review and Search Strategy (CRSS) meeting. This significantly saves down-stream labor because the CRSS meeting is the first assessment meeting in the Section 5 chemical review process.

In late 1984, Charles Auer, Paul Bickart, David Klauder, and Justin Powell held a series of informal meetings to formulate new criteria that might permit more substances to be

dropped at the CRSS meeting. These meetings did not produce any useful criteria because it was difficult to formulate such criteria without actual examples. Subsequently, Justin Powell and Paul Bickart initiated an effort to develop criteria based on actual case experience.

The strategy consisted of tentatively identifying potential drop cases at the CRSS meeting. To gain another perspective, we also asked the Structure/Activity Team (SAT) to independently identify cases it wished ICB had dropped before the SAT meeting. The scope of tentative drops was not limited to polymers, although, as might be expected, most of the examples are polymers. At the CRSS meeting, we used professional judgment, knowledge, and experience to identify substances that seemed destined to drop at the Focus meeting. Part of our strategy was to develop criteria by evaluating the regulatory fate of actual examples that were identified as potential drops.

In the initial phase of the work, we identified about 100 such examples. This consumed about six months. During this time, we reviewed about 1000 substances and made regular CRSS drops as usual, i.e., we identified tentative drops along with the regular drops.

B. Old Criteria and Framework

Our original criteria were applicable only to polymers. "Polymers" are not defined in TSCA nor in the PMN Rule, so the criteria were applicable to substances judged by CRSS to be polymers.

In order for CRSS to drop a polymer previously, it must have met four formal conditions:

1. it must be a member of one or more "droppable" classes of polymers;
2. it must contain no more than a certain amount of low-molecular-weight oligomers;
3. it must not be water-soluble; and
4. it must not be a "reactive prepolymer."

There was also an informal condition: there should not be a reason to continue the review based on professional judgment or review experience.

A form certified that the polymer met the formal conditions is attached to the ICB Chemistry Report; see the Appendix, Fig. 1.

There were eight droppable classes of polymers, as interpreted by CRSS: polyesters, polyamides, polyacrylates, polyurethanes, polyolefins, polysulfones, polyethers, and polysiloxanes.

The oligomer-content criterion specified that the substance contained no more than five weight percent of species with molecular weight less than 500. (As interpreted by CRSS, this applied only to the product and did not include residual starting materials.) This criterion could have been met either on the basis of information supplied by the manufacturer, or on the basis of a judgment by the CRSS chemists. This professional judgment, in turn, may have been based upon property data supplied by the submitter or upon the CRSS chemists' knowledge

of the class of chemicals or knowledge of the characteristics of molecular weight distributions.

The water-solubility criterion stated that the polymer "is not reasonably anticipated to be water-soluble." Commonly, this was taken to mean "less than one weight percent soluble," but typically CRSS interpreted this criterion more stringently. We considered solubility in water down to the level of a hundred or even ten parts per million, especially when polymers with appreciable numbers of amine groups, other potentially cationic groups, or cationic groups were involved. On the other hand, CRSS did not usually equate "dispersibility" with solubility, and many substances reported by submitters as "water-dilutable" were not considered by CRSS to be water-soluble. This was typically the case with acrylic latices, for example.

"Reasonably anticipated" is a finding that can be made either by the submitter or by CRSS. The meaning of "reasonably anticipated" is that a person knowledgeable in chemistry would expect a given physical or chemical composition or characteristic to occur, based on such factors as the nature of the precursors used to manufacture the polymer, the type of reaction, the type of manufacturing process, the products produced in polymerization, the intended uses of the substance, or associated use conditions.

The non-reactivity criterion stated that the polymer "is not judged to be a reactive prepolymer," that is, it does not contain reactive functional groups. As CRSS interpreted this, ordinary alcohols and carboxylic acids, even if intended for further reaction (as, for example, in a polyester polyol

intended as a polyurethane precursor) were considered non-reactive. Amine groups were also considered non-reactive (although they are considered reactive in the Polymer Exemption). Acrylate and methacrylate esters were considered as reactive although typically they require free-radical initiators, light, or ionizing radiation for reaction. Phenolic resins were generally considered as reactive (the reactive sites are unsubstituted positions ortho and para to the hydroxyl groups). Alkoxysilanes were considered reactive, but the reactivity is markedly higher when the group is methyl or ethyl than when it is propyl or larger than propyl. Blocked isocyanates (typically capped with an oxime, a phenol, or an amide) were also considered as reactive although they are made in order to reduce their reactivity relative to the unblocked form and typically require elevated temperatures, with or without catalysis, for further reaction.

The wording of this criterion may have suggested that polymers that are not prepolymers could have had reactive functional groups and still have been dropped. No such implication was intended. Moreover, the examples of functional groups considered reactive or nonreactive were not intended to be limiting. Any atom or substructure could be construed as reactive. Functional groups were also considered in their molecular context: contrast the hydroxyl group in a saturated aliphatic hydrocarbyl alcohol to the hydroxyl group in a methylolurea (the latter, but not the former, was considered reactive).

C. Interim Criteria

Several modifications to the criteria outlined above have been in effect for years. The criteria used on an interim basis were applicable only to materials recognized by CRSS that were judged to meet the definition of polymer in the Polymer Exemption Rule. Materials of comparable molecular weights that are not polymers were not treated as polymers by CRSS even though the same criteria might be appropriately applied.

1. With the concurrence of the Premanufacture Notice Management Branch, the oligomer-content criterion was being applied somewhat flexibly. For example, if the submitter indicated that the portion of the substance with molecular weight less than 500 is somewhat greater than five weight percent, the amount reported may have been judged to be essentially the same as five weight percent. This judgment was permissible if the portion with molecular weight less than 1000 was reasonably low and the polymer was a member of a class of compounds that almost never cause concern (e.g., polyesters). This judgment was noted on the drop form when it was made.
2. An exception to the reactive-functional-group criterion described above was in effect with respect to the acrylate and methacrylate groups: as long as the polymer contains no more than two

weight percent below a molecular weight of 500, the polymer could have been dropped even though it contained those specific reactive functional groups. (This relaxed criterion was an outcome of the Structure/Activity Team's judgment that high molecular weight polyfunctional acrylates or methacrylates are unlikely to produce carcinogenic or mutagenic effects.)*

3. Although the reactive-functional-group criterion does not specify any acceptable level for such groups, a threshold was applied. The threshold was the one used in the Polymer Exemption Rule: an equivalent weight per reactive function group of 10,000 or more. (This means that a substance was dropped from consideration if there was one reactive functional group gram-equivalent or less in 10,000 grams of the chemical substance.)
4. Finally, certain groups were excluded from consideration under the criterion above. Any level of such excluded reactive functional groups would not have prevented a substance from being

*In the review of a draft of this document, we learned that the Health Effects Review Division takes number-average molecular weight into consideration. Their criteria for acrylates and methacrylates had included a minimum average molecular weight of 2000. We suggested that two levels be set for oligomer content, to assure a relatively low level of small molecules rather than using the molecular weight criterion. We proposed setting a corresponding value for the permissible weight percent below 1000, in addition to the criterion of two percent below 500. Later, HERD decided to place acrylates and methacrylates under the equivalent weight concept. This resolved the matter.

dropped. These excluded groups included amines, carboxylic acid groups, aliphatic hydroxyl groups, unconjugated olefinic groups that are considered "ordinary," butenedioic acid groups, or conjugated olefinic groups in naturally-occurring fats, oils, and carboxylic acids. (Except for amines, which are covered under provisions for potentially cationic substances, these groups were the ones excluded from the corresponding criterion in the Polymer Exemption Rule.)

III. Results and Discussion

A. Case Relevance to Criteria

Of the 106 cases identified in this study, 104 (98 percent) were eventually dropped. The status of these 106 cases is that 96 had their new chemical review terminated at the Focus Meeting (drops or grants), four were withdrawn, and six entered Standard Review. One of the withdrawn cases was a duplicate submission that had been previously reviewed and dropped at Focus. The other three withdrawn cases were resubmitted as different types of cases. Two of these were dropped at CRSS and one was dropped at Focus. Four of the cases in Standard Review were later dropped and two were in suspension. For the purposes of this study, we presume that these latter cases are false negatives. These data are shown in Table I of the Appendix.

In developing drop concepts, we found that 79 (76 percent)

of the 104 cases which were ultimately dropped (and neither of the two false negatives) could be formally dropped using both reasonable modifications of our present criteria and framework as well as newer concepts for criteria that did not fit our present framework. To expedite the introduction of certain concepts which could be implemented sooner, we delayed the development of newer drop concepts and a new framework.

The criteria we recommend would drop 48 (46 percent) of the 104 cases that ultimately dropped or 61 percent of the cases that both the presently recommended criteria and the future criteria would be likely to drop. These data are shown in Table 2 in the Appendix.*

In examining these data, several points should be noted. These criteria have not been applied to cases that were not tentatively identified as drops. This could have resulted in more drops. To some extent, these statistics are also dependent on interpretations we made where data were lacking. Finally, the accuracy of extrapolation of these results to future new chemical submissions is dependent on how well substances are characterized in the submissions and how the characteristics of future submission will vary.

*This computation is based upon an analysis performed using a draft version of the new criteria. The current proposal includes changes that may act in opposing directions. The net result, in our opinion, is likely to be either no change or a modest increase in the incidence of drops.

B. Recommendations for New Criteria and Implementation

Examining the cases identified as tentative drops, we infer some general approaches for dropping additional cases at CRSS with reasonable assurance that they would be dropped if they proceeded to the Focus meeting. All of the proposed criteria are governed by one or more of the following principles:

1. Permissive criteria may be expanded by adding more classes of chemicals. Such criteria are based on the intrinsic lack of toxicity of the chemicals of a given class. Thus, for example, aromatic polythioethers may be added to the list of permissible polymer types.

2. Restrictive criteria may be loosened in several ways.

   a. Absolute restrictions may be replaced by acceptable threshold conditions. For example, the criterion of water-insolubility can be replaced by a maximum permitted level of water-solubility, or as in the interim criteria, a level of no more than one gram-equivalent of reactive functional groups per 10,000 grams of polymer might replace the criterion of nonreactivity.

   b. Restrictions may be loosened by applying selective numerical criteria to subcategories of the restriction. For example, a greater concentration might be permitted for certain reactive functional groups than for others.

c. Restrictions may be weakened by redefinition. For example, groups which chemically react only at elevated temperatures might be redefined as nonreactive rather than as reactive.

d. Restrictions may be more narrowly defined. For example, instead of requiring that a polymer be insoluble in water, the criterion could restrict the exclusion to water-soluble polymers of the cationic or sulfonated aromatic anionic types.

The framework we propose for implementation is essentially the same scheme that was in use. One overall modification is to state explicitly that these criteria can be applied only to well-defined polymers. This modification recognizes that the identities of chemicals reflect complex industrial processes, inherent diversity in the arrangement and bonding of chemical structures, and the multicomponent nature of most industrial chemicals.

Chemical data supplied under Section 5 of TSCA may conform to the regulatory requirements and constitute what is "reasonably ascertainable"; however, these data may not be adequate for judgments. We can not implement criteria if we must explicitly or implicitly presume particular knowledge of composition, identity, analysis, or properties. Thus, chemical substances that cannot be sufficiently well defined will not be dropped. This framework also explicitly adopts the Polymer Exemption definition for "polymer."

Below we propose four criteria that we think can be incorporated into our current process without protracted

additional development. Review shall not be stopped unless all four of these criteria are satisfied:

1. Polymer Category Expansion

   Several new types of polymers have been submitted since the drop policy was established. We believe that some of these can be included now. The droppable classes of polymers, as interpreted by CRSS, are expanded as follows:

   (1) polyesters (this category includes alkyd resins and polycarbonates);

   (2) polyamides and polyimices;

   (3) polyacrylates (addition polymers of acrylates, acrylonitrile, and acrylamide, as well as the corresponding methacrylate derivatives are in this category);

   (4) polyurethanes and polyureas;

   (5) polyolefins (including polymers of dienes, vinyl and vinylidene compounds, styrene derivatives, and allyl derivatives);

   (6) aromatic polysulfones;

   (7) polyethers (including acetal resins and many epoxy derivatives); and

   (8) polysiloxanes (including silsesquioxanes; modification by silicates is also a permissible variation);

   (9) polyketones;

   (10) aromatic polythioethers;

(11) polymeric hydrocarbons (not derived from olefins);

(12) phenol-formaldehyde copolymers.

2. Oligomer Content Expansion

The maximum permissible levels of oligomer present in a polymer are 10 weight percent for polymer molecules with molecular weight less than 500 and 25 weight percent for polymer molecules with molecular weight less than 1000.

The use of two points in the molecular weight distribution recognizes the error in such determinations and gives a rough idea of the slope of the distribution near the low end. The values chosen are consistent with one another on the basis of data gathered for the Polymer Exemption.

3. Permissible Ionic Character and Solubility

By analogy with the polymer exemption, water-solubility would not be grounds for failing to drop an otherwise droppable polymer. However, in developing a new criterion, we recognized that the relationship between ionic character and water-solubility is complex. Originally, we proposed that only if the polymer were cationic, potentially cationic, or an aromatic sulfonate type of anionic, could water-solubility consign the polymer to further review. If the concentration of ionic groups of concern was not great, then some degree of water-

solubility could be acceptable. Other types of anionic and nonionic water-soluble polymers would not be prevented from being dropped by this new criterion. Moreover, if 5000 is considered an appropriate threshold for such charged substructures, we believe that a water-solubility threshold would would not be exercised often. Thus, the following is revision of the water-solubility criterion.

Polymers satisfy this criterion if one of the following conditions are met.

The polymer molecules of the substance contain relatively few covalently-linked substructures that are, or can be reasonably anticipated to become

a. anionic aromatic sulfonate substructures such that the polymer has an equivalent weight equal to or less than 5000 for such charged substructures or

b. positively charged in a natural aquatic environment and such that the polymer has an equivalent weight equal to or less than 5000 for such charged substructures.

4. Reactive Functional Group Thresholds

Polymers would satisfy this criterion if one of the following conditions are met.

The polymer molecules of the substance

a. contain, or can resonably be anticipated to contain

(1) no reactive functional groups (atoms or associated groups of atoms that undergo, or can be reasonably anticipated to undergo, facile chemical reaction) or

(2) only the following excluded reactive functional groups:

thiols, blocked isocyanates (other than acetoxime- and methyl ethyl ketoxime-blocked isocyanates), amines, carboxylic acid groups, aliphatic hydroxyl groups, unconjugated olefinic groups that are considered "ordinary," butenedioic acid groups, and conjugated olefinic groups in naturally-occurring fats, oils, and carboxylic acids or

b. have, or can be reasonably anticipated to have, a total equivalent weight for all reactive functional groups present that is no less than:

(1) 5000 if any reactive functional group is present that is not listed in Table 3;

otherwise,

(2) the relevant minimum value listed in Table 3 if only one kind of listed reactive functional group is present; or,

(3) the highest minimum value listed in Table 3 using a calculated total functional group-equivalent weight if more than one kind of listed functional groups is present, (for detail and the calculation, see Table 3 and the note in Appendix E.)

The former interim criteria that had been applied to acrylates and methacrylates are replaced by equivalent weight minima for these groups. (Discussed under Interim Criteria 3.)

Reactive functional groups named in Table 3 include: acid halides; acid anhydrides; acrylates; aldehydes, hemiacetals, methylolureas, -amines, and -amides (and their hydrocarbyloxy-methylene analogs); alkoxysilanes; allyl ethers; aziridines; carbodiimides; conjugated olefins (except those olefinic groups present in naturally-occurring fats, oils, and carboxylic acids); cyanates; epoxides; halosilanes and hydrosilanes; hydrazines; imines; isocyanates and their acetoxime- and methyl ethyl ketoxime-blocked analogs; isothiocyanates; alpha- and beta-lactones; methacrylates; unsubstituted positions ortho- or para- to phenol; and vinyl sulfones (and their analogous precursors).

Certain groups previously considered as reactive are redefined here as nonreactive. These include thiols and blocked isocyanates (other than acetoxime- and methyl ethyl ketoxime-blocked isocyanates). The groups excluded in our interim criteria would also be excluded under our new criteria: amines, carboxylic acid groups, aliphatic hydroxyl groups, unconjugated olefinic groups that are considered "ordinary," butenedioic acid

groups, or conjugated olefinic groups in naturally-occurring fats, oils, and carboxylic acids. (For example, allyl ether, vinyl ether, allyl silane, and vinyl silane groups are not considered ordinary olefinic groups.)

These criteria may be overridden by professional judgment when special concerns arise. If the CRSS meeting chairperson or a consensus of ICB chemists present considers it imprudent to drop a substance, review will continue. In particular, HERD has requested that ICB exercise its professional judgement if there seemed to be a likely inhalation exposure to polymer dusts or aerosols. Many submissions that concern polymers that are, or could reasonably be, solids contain insufficient information to make this judgment. We propose to judge on the basis of submitted information only.

Any OTS assessor may question a CRSS drop by referring it through his or her Section Chief (or higher) to the ICB New Chemicals Section Chief (or higher) for review and redetermination. ICB plans to periodically review these criteria and revise them in light of a continuing evaluation of the decisions made at CRSS.

We plan to incorporate the determination that a substance has or has not been dropped into the Chemistry Report format instead of optionally adding a separate form. The instructions will require a positive or negative drop finding, date, CRSS chair's signature, and criteria reference. We do not plan to document specific subparts of criteria met or not met because this has not been used.

C. Future Work

In the course of this work, we have suggested modified criteria and new concepts that could permit more CRSS drops in the future. These new concepts go beyond simple modifications of the current scheme, and developing them would have delayed the significant improvements offered by the modifications.

Briefly, future criteria of "safeness" fall into three categories: those based on the safeness of precursor substances; those based on general recognition of the safeness of the substance itself; and those based on safeness that is dependent on physical (usually macromolecular) properties. Precedents for and examples of these concepts include the "polyester" condition of the Polymer Exemption, the FDA GRAS list, and the generalization that large, inert molecules are rarely bioabsorbable.

These future criteria need not be limited to the evaluation of polymers. For example, limits to oligomer levels could be used to sort substances into groups containing different levels of low molecular weight species. Criteria could then be designed that would apply only for substances of low, high, or intermediate molecular weight.

Integrating future criteria with existing ones will require a framework for making decisions that is more flexible, more reliable, and more efficient than our current approach: a framework that can accommodate different kinds of criteria and different relationships among them. To bolster reliability, we

would require that only well-characterized and -defined chemical substances could be eligible for a drop, and that the criteria, framework, and procedures themselves would be continuously subject to professional judgment and review.

Our core concept for a future framework has three decision levels, and at each level are criteria that determine the eligibility of a substance for termination of review. Some of these criteria have priority over others at the same decision level, and each level has priority over the succeeding one. Substances not addressed at one level may be considered in the next. In the first level, substances are sorted into three categories: those that are clearly not droppable; those that are clearly droppable; and all the rest. Substances in the third category are sorted at the second level by oligomer content, and further drops may be possible at this level. Finally, at the third level, each group of substances identified at the second level is judged according to custom-made criteria.

To develop the new criteria, we will prepare lists of acceptable substances, precursors of substances, and properties; devise a relationship for estimating oligomer content; and define conditions for establishing the acceptable ranges for various properties. It will require considerably more work to find ways to represent substances not only as specific chemical identities but also as members of chemical categories or families, and establishing various conditional levels will require gathering data to support a rationale. Finally, we will need general concurrence on the levels and the approach.

Appendix

A. Methods

In May of 1985, we decided to identify about 100 PMN's and Polymer Exemption Notices that could not have been dropped using our current criteria and from which we thought we could derive acceptable, expanded criteria. We identified these cases in two ways: first, we identified at the CRSS meeting those cases we thought would be dropped at the Focus meeting; second, we requested that the Structure/Activity Team (SAT) independently refer cases to us that they wished we had dropped at CRSS. We manually recorded these as "CRSS tentative drops" and "SAT tentative drops" respectively. During the time we collected these examples, the Chemical Control Division extended the applicability of CRSS drops to Low Volume Exemption Notices and to Test Market Exemption Applications, and we also included these kinds of cases within the scope of our survey. By November, 1985, we had identified 106 cases, and we stopped this phase of work.

We then began to compile data for the substances reported in these cases, assigning code numbers to the cases to protect TSCA Confidential Business Information. Data gathered include the case number, salient chemical identity information, whether or not the case was identified at CRSS or SAT, ratings from the SAT and Exposure Assessment Meeting (EXAM), and dispositions from the Focus Meeting. Where supplementary data were needed, the case

file was checked to verify or to obtain more information, and, when necessary, data bases were searched to obtain updated disposition information. The non-CBI information is provided as Table 1 in the Appendix; a CBI version is available.

We evaluated these examples by considering how the substances failed to satisfy existing criteria and by formulating criteria that could permit the substances to drop. These tentative criteria were further characterized and reconsidered for what they might imply beyond the examples in hand, and this led in turn to the proposed criteria modifications. The results of this analysis are presented in Table 2 in the Appendix.

We integrated the proposed criteria into an expanded version of the framework we were using. Our evaluation also led to new criteria that will require further development, including an alternative way to apply the criteria, and an alternative framework for using new kinds of criteria.

B. Data

For a number of reasons, our sample is unlikely to be representative. One reason is that it is small. ICB has reviewed over eleven thousand submissions. In this study we identified 106 cases out of 941 valid submissions received in sequence between May and November, 1985. We know from experience that during this time we received an anomalous proportion of at least one class of substances. Moreover, while this effort was in progress, exemption submissions for test marketing and low-

volume chemicals became subject to regular CRSS termination criteria for the first time. This introduced more heterogeneity into our sample. The statistics we have are also incomplete because CRSS drop data are not readily available for exemption submissions: OTS data bases contain these data only for PMN's.

During the time the sample cases were selected, the Agency received 999 submissions of which 941 (94 percent) were valid, including 675 (72 percent) valid PMN's of which 145 (21 percent) were CRSS drops. This is roughly comparable with all cases in FY '85: 1858 submissions, 1774 (95 percent) valid submissions, 1462 (82 percent) valid PMN's, and 264 (18 percent) CRSS drops. The lower percentage of PMN's, for the period studied compared to the year, reflects the submission of increased numbers of new kinds of exemption notices in lieu of PMN's for the period.

Of the 106 cases we identified, 91 (86 percent) were PMN's, 13 (12 percent) were polymer exemptions, and one each (0.9 percent each) were test market and low-volume submissions. ICB tentatively dropped 98 cases (92 percent); SAT tentatively dropped 61 cases (58 percent). Of the cases on our list, 50 percent were tentatively dropped by both ICB and SAT.

In all, 104 of 106 cases (98 percent) were ultimately dropped. These cases would have raised the number of CRSS drops during the period of the study to at least 249 (26 percent). We estimate that 70 additional chemicals (mostly polymer exemptions) could have been added if all exemption cases had been subject to tentative drops. Thus, at most, CRSS drops could be expanded to about one-third of valid cases overall.

C. Figure

Figure 1.

Current Drop Form, page 27

Figure 1

Date of CRSS meeting: contains CBI? yes[] no[]

JUSTIFICATION FOR TERMINATING

FURTHER ASSESSMENT OF

P[] Y[] L[] T[] 8 -_____

The substance is a polymer that satisfies the following criteria for terminating assessment:

A. The substance is member of the following class(es):

[] polyester (including alkyd and polycarbonate)
[] polyamide or polyimide
[] polyacrylate, -acrylonitrile, or -acrylamide
[] polyurethane or polyurea
[] polyolefin, -styrene, or other polyvinylic
[] polysulfone
[] polyether (including acetal)
[] silicone

B. The substance has been determined by the CRSS team to contain no more than 5% by weight of species with molecular weight less than 500 daltons on the basis of:
1. information supplied by the submitter []
2. professional judgment of the CRSS team []

C. The substance is not designed to be water-soluble []

D. The substance is not a reactive prepolymer []

D. Tables

Table 1
Disposition of Tentative Drops

No.	CTD	STD	HEALTH	ECO	OCC. EXP.	CON. EXP.	ENVIR. EXP.	FOCUS DISP.
1	X	X	1	1	1	1	1	Drop
2	X	X	1	1	1	1	1	Drop
3	X	-	1	1-2	1	1	1-2	Drop
4	X	-	1	1	2	1	1	Drop
5	X	-	1	1	1	1	1	Drop
6	X	-	1	1	1	1	1	Drop
7	X	-	1	1	1-2	1	1	Drop
8	X	X	1	1	2	1	1	Drop
9	X	-	1	1	1	1	1	Drop
10	X	X	1	1	1	1	1	Drop
11	X	-	1	1	1	1	1	Drop
12	X	-	-	-	-	-	-	Drop
13	X	-	1	1	-	-	-	Drop
14	X	-	1	1	1	1	1	Drop
15	X	-	1	1	1	1	1	Drop
16	X	-	1	1	1	1	1	Drop
17	X	-	1	1-2	1	1	1	Drop
18	X	X	1	1	2	1	1	Drop
19	X	X	1	1	2	1	1	Drop
20	X	-	1	1	2-3	1	1	Drop
21	X	-	1	1	2-3	1	1	Drop
22	X	-	1	1	2-3	1	1	Drop
23	X	X	1	1	2	1	3	Drop
24	X	X	1	1	2	1	3	Drop
25	X	X	1	1	2	1	3	Drop

No.	CTD	STD	HEALTH	ECO	OCC. EXP.	CON. EXP.	ENVIR. EXP.	FOCUS DISP.
26	X	X	1	1	1-2	1	1	Drop
27	X	X	1	1	1	1	1	Drop
28	X	X	1	1	2	1	1	Drop
29	X	X	1	1	2	1	1	Drop
30	X	X	1	1	2	1	1	Drop
31	X	X	1	1	2	1	1	Drop
32	X	X	1	1	2	1	1	Drop
33	X	X	1	1	2	1	1	Drop
34	X	X	1	1	1	1	1	Drop
35	X	X	1	1	1	1	1	Drop
36	X	X	1	2	1	1	1	Drop
37	X	X	1	1	2	1	1	Drop
38	X	X	1	1	-	-	-	Drop
39	X	-	-	-	-	-	-	Drop
40	X	-	-	-	-	-	-	Drop
41	X	-	1	1	1	1	1	Drop
42	X	X	1	1	1-2	1	1	Drop
43	X	-	1	1	2	1	1	Drop
44	X	-	1	1	2	1	1	Drop
45	X	-	1	1	2	1	1	Drop
46	X	-	1	1	2	1	1	Drop
47	X	-	1	1	2	1	1	Drop
48	X	-	1	1	2	1	1	Drop
49	X	-	1	2	1	1	1	Drop
50	X	-	1½	1	2	1	1	Drop
51	X	-	1½	1	2	1	1	Drop
52	X	X	1	1	1	1	1	Drop

No.	CTD	STD	HEALTH	ECO	OCC. EXP.	CON. EXP.	ENVIR. EXP.	FOCUS DISP.
53	X	X	1	1	2	1	1	Drop
54	X	X	1	1	1-2	1	1	Drop
55	X	-	1-2	1	2	1	1-2	Drop
56	X	X	1	1	2	1	1	Drop
57	X	X	1	1	2	1	1	Drop
58	X	X	1-2	1	2-3	1	1	Drop
59	X	X	1-2	1	2-3	1	1	Drop
60	X	-	1	2	1	1	1-2	SR
61	X	-	1	1	-	-	-	Drop
62	X	X	1	1	1	1	1	Drop
63	X	X	1	1	-	-	-	Drop
64	X	-	-	-	-	-	-	Drop
65	X	-	-	-	-	-	-	Drop
66	X	-	-	-	-	-	-	Drop
67	X	-	1	1	1-2	1	1	Drop
68	X	-	-	-	-	-	-	Drop
69	X	X	1	1	1-2	1	1	Drop
70	X	-	1	2	1-2	1	1	Drop
71	X	X	1	1	1	1	1-2	Drop
72	X	-	1-2	1	1	1	1	Drop
73	X	-	1	1	2-3	1	1	Drop
74	X	X	1	1	1	1	1	Drop
75	X	X	1	1	2	1	1	Drop
76	X	-	2	3	1-2	1	1	Drop
77	X	X	1	2	2	1	1	Drop
78	X	X	1	1	2-3	1	1	Drop
79	X	X	1	1	1	1	1	Drop

No.	CTD	STD	HEALTH	ECO	OCC. EXP.	CON. EXP.	ENVIR. EXP.	FOCUS DISP.
80	X	X	1	1	1	1	1	Drop
81	X	-	1	1	1-2	1	1-3	Drop
82	X	-	1	1	1	1	1	Drop
83	X	-	1	1-2	1-2	1	1	Drop
84	X	X	1	1	-	-	-	Drop
85	X	X	1	1	-	-	-	Drop
86	X	-	1	1	2	1	1	Drop
87	X	-	1	2	-	-	-	Drop
88	X	-	1	1	-	-	-	Drop
89	X	-	1	2	1	1	1-2	SR
90	X	-	1	1	1	1	1	Drop
91	X	-	1-2	1	2-3	1	1	Drop
92	X	-	1-2	1	2-3	1	1	Drop
93	X	X	1	1	2	1	1	Drop
94	X	X	1	1	2	1	1	Drop
95	X	-	1	1	1	1	1	Drop
96	X	X	1	1	2-3	1	1	Drop
97	X	X	1	1	2-3	1	1	Drop
98	X	X	1	1	-	-	-	Drop
99	X	X	1	1	-	-	-	Drop
100	X	-	1	1	2	1	1	Drop
101	X	-	1	1	2	1	1	Drop
102	X	X	1	1	1-2	1	1	Drop
103	X	X	1	1	1-2	1	1	Drop
104	X	X	1	1	1-2	1	1	Drop
105	X	X	1	1	1	1	1	Drop
106	X	X	1	1	1	1	1	Drop

Key to Case Criteria Analysis
for Table 2

Item	Description
Case	"dummy" number of submission to protect CBI
1-4C	1 means the numbered modified criterion is met
F1-F3	1 means the numbered future criterion is met
D1	1 means that modified criteria 4B-1, -2, -3, and -4C are met, 0 means the case does not satisfy all four criteria
D2	1 means that the case satisfies future criterion F1, F2, or F3, 0 means no future criterion is met
D3	1 means that either D1 or D2 are satisfied, 0 means that neither D1 nor D2 are satisfied

Since this analysis was completed, the incorporation of comments has simplified the structure of the criteria; therefore, the table refers to subcriteria that have been eliminated. Please refer to the April 6, 1987, draft of this document for details of the earlier criteria.

Table 2

Case Criteria Analysis

CASE	1	2	3A	3B	3C	3D	4A	4B 1	4B 2	4B 3	4C	F1	F2	F3	D1	D2	D3
1	1	1				1	1								1	0	1
2	1	1				1	1							1	1	1	1
3	1	1	1				1					1			1	1	1
4	1	1	1				1							1	1	1	1
5	1	1					1								0	0	0
6	1	1					1								0	0	0
7	1	1	1						1						1	0	1
8				1									1		0	1	1
9	1	1	1						1						1	0	1
10	1	1	1								1				1	0	1
11	1	1	1						1						1	0	1
12	1		1				1								0	0	0
13	1	1	1				1								1	0	1
14	1		1				1								0	0	0
15	1	1	1				1								1	0	1
16	1	1	1				1								1	0	1
17	1		1				1								0	0	0
18	1		1				1								0	0	0
19	1		1				1								0	0	0
20				1									1		0	1	1
21				1									1		0	1	1
22				1									1		0	1	1
23				1									1		0	1	1
24				1									1		0	1	1
25				1									1		0	1	1
26															0	0	0
27	1	1	1												0	1	1
28				1									1		0	1	1
29				1									1		0	1	1
30				1									1		0	1	1
31				1									1		0	1	1
32				1									1		0	1	1
33				1									1		0	1	1
34	1	1	1									1			1	0	1
35	1	1	1							1					1	0	1

Table 2

Case Criteria Analysis

								4B									
CASE	1	2	3A	3B	3C	3D	4A	1	2	3	4C	F1	F2	F3	D1	D2	D3
36	1	1	1				1					1			1	1	1
37	1	1	1						1						1	0	1
38	1		1				1								0	0	0
39	1	1				1	1								1	0	1
40	1	1				1	1								1	0	1
41	1	1				1	1								1	0	1
42	1	1	1						1						1	0	1
43	1	1	1								1				1	0	1
44	1	1	1												0	0	0
45	1	1	1												0	0	0
46	1	1	1												0	0	0
47	1	1	1												0	0	0
48	1	1	1											1	0	1	1
49	1	1	1												0	0	0
50	1	1	1				1					1			1	1	1
51	1		1				1					1			0	1	1
52			1				1						1		0	1	1
53	1	1	1				1						1		1	1	1
54	1	1					1								0	0	0
55	1	1	1				1					1			1	1	1
56	1		1				1					1			0	1	1
57	1	1	1				1								1	0	1
58	1	1		1					1						1	0	1
59	1	1		1					1						1	0	1
60	1	1					1								0	0	0
61	1		1				1						1		0	1	1
62			1				1					1			0	1	1
63	1	1	1				1					1			1	1	1
64	1	1		1			1								1	0	1
65	1	1		1			1								1	0	1
66	1	1		1			1								1	0	1
67	1		1				1								0	0	0
68	1		1				1					1			0	1	1
69	1	1		1			1								1	0	1
70	1	1					1								0	0	0

Table 2

Case Criteria Analysis

								4B									
CASE	1	2	3A	3B	3C	3D	4A	1	2	3	4C	F1	F2	F3	D1	D2	D3
71	1	1					1					1	1		0	1	1
72	1	1	1				1							1	1	1	1
73	1	1		1			1							1	1	1	1
74	1		1				1					1	1		0	1	1
75	1	1	1				1								1	0	1
76			1				1								0	0	0
77			1				1								0	0	0
78	1	1				1	1								1	0	1
79	1	1	1				1					1			1	1	1
80	1	1	1				1					1			1	1	1
81							1								0	0	0
82	1	1					1								0	0	0
83	1		1				1					1			0	1	1
84	1	1		1			1								1	0	1
85	1	1	1				1						1		1	1	1
86	1	1	1				1						1		1	1	1
87	1	1				1	1								1	0	1
88	1	1		1			1								1	0	1
89	1						1								0	0	0
90	1	1					1								0	0	0
91	1	1	1				1								1	0	1
92	1	1	1				1								1	0	1
93	1		1						1						0	0	0
94	1	1	1												0	0	0
95			1				1					1	1		0	1	1
96	1	1	1												0	0	0
97	1		1				1						1		0	1	1
98	1	1	1				1						1		1	1	1
99	1	1	1				1						1		1	1	1
100	1	1	1						1					1	1	1	1
101	1	1	1						1						1	0	1
102	1		1				1						1		0	1	1
103	1		1				1					1	1		0	1	1
104	1		1				1					1	1		0	1	1
105			1				1					1	1		0	1	1
106			1				1					1	1		0	1	1
SUM	84	65	66	22	0	7	68	0	11	0	3	18	30	6	48	48	79
%	79	61	62	20	0	6.6	65	0	10	0	2.8	17	28	5.6	45	45	74

Table 3.

Allowable Thresholds for Reactive Functional Groups

Name	Substructure	Minimum Permissible Equivalent Weight
Acid halides		1000
Acid anhydrides		1000
Acrylates		5000
Aldehydes		1000
Alkoxysilanes	(alkyl > C_2)	1000
	(alkyl = Me or Et)	5000
Allyl ethers		1000
Aziridines		5000
Carbodiimides		5000
Conjugated olefins		1000
Cyanates		1000
Epoxides		1000
Halosilanes		5000
Hydrazines		5000
Imines		1000
Isocyanates		5000
Isothiocyanates		5000
alpha-Lactones, beta-Lactones		5000
Methacrylates		5000
Unsubstituted position ortho- or para- to phenol		1000
Vinyl sulfones		5000

E. Note on Weighted-average Calulation

A polymer containing different reactive functional groups $g_1, g_2, \ldots, g_n$, with corresponding group-equivalent weights $w_1, w_2, \ldots, w_n$, (from Table 3) has wt_{tot}, a total reactive functional group equivalent weight, equal to the inverse of the sum of the inverse w_n's:

$$wt_{tot} = \frac{1}{1/w_1 + 1/w_2 + \ldots + 1/w_n}$$

The threshold applicable to w_{tot} is the <u>largest</u> of any of the individual group thresholds. For a polymer containing reactive functional groups to be dropped, w_{tot} is not permitted to be <u>smaller</u> than the <u>largest</u> of the individual <u>minimum</u> equivalent weights for any of the groups present. This approach allows for synergistic effects, but limits the extent of such effects to that which would occur if all the groups were the same as the most hazardous group present.

For example, a polymer with an acrylate equivalent weight of 10,000 (Table 3 threshold: 5000) and an epoxide equivalent weight of 5000 (Table 3 threshold: 1000) would have a total reactive functional group equivalent weight of 1/[(1/10,000) + (1/5000)], or 3333. Thus the polymer exceeds the reactive functional group criterion because wt_{tot} is less than the more restrictive acrylate threshold level.